What is claimed is:

1. A molecule or molecular complex comprising at least a portion of an *S. aureus* peptide deformylase or an *S. aureus* peptide deformylase-like active site comprising amino acids Gly58, Gly60, Leu61, Gln65, Glu109 , Gly110, Cys111, Leu112, Ile150, His154, Glu155, and His158, the active site being defined by a set of points having a root mean square deviation of less than about 0.35 Å from points representing the backbone atoms of said amino acids as represented by structure coordinates listed in Table 1.

2. The molecule or molecular complex of claim 1 further comprising a coordinated metal ion selected from the group of metals consisting of Fe, Zn, Ni and combinations thereof.

3. The molecule or molecular complex of claim 2, wherein the metal ion is coordinated by the amino acids Cys111, His154, and His158.

4. A molecule or molecular complex comprising at least a portion of an *S. aureus* peptide deformylase or an *S. aureus* peptide deformylase-like active site comprising amino acids Arg56, Ser57, Gly58, Val59, Gly60, Leu61, Gln65, Leu105, Pro106, Thr107, Gly108, Glu109 , Gly110, Cys111, Leu112, Asn117, Tyr147, Ile150, Val151, His154, Glu155, and His158, the active site being defined by a set of points having a root mean square deviation of less than about 0.8 Å from points representing the backbone atoms of said amino acids as represented by structure coordinates listed in Table 1.

5. The molecule or molecular complex of claim 4 further comprising a coordinated metal ion selected from the group of metals consisting of Fe, Zn, Ni and combinations thereof.

6. The molecule or molecular complex of claim 5, wherein the metal ion is coordinated by the amino acids Cys111, His154, and His158.

7. A molecule or molecular complex that is structurally homologous to an *S. aureus* peptide deformylase molecule or molecular complex, wherein the *S. aureus* peptide deformylase molecule or molecular complex is represented by structure coordinates listed Table 1.

8. The molecule or molecular complex of claim 7 further comprising a coordinated metal ion selected from the group of metals consisting of Fe, Zn, Ni and combinations thereof.

9. A scalable three-dimensional configuration of points, at least a portion of said points derived from structure coordinates of at least a portion of an *S. aureus* peptide deformylase molecule or molecular complex listed in Table 1 and having a root mean square deviation of less than about 1.4 Å from said structure coordinates.

10. A scalable three-dimensional configuration of points, all of said points derived from structure coordinates of an *S. aureus* peptide deformylase molecule or molecular complex listed in Table 1 and having a root mean square deviation of less than about 1.4 Å from said structure coordinates.

11. The scalable three-dimensional configuration of points of claim 9 wherein at least a portion of the points derived from the *S. aureus* peptide deformylase structure coordinates are derived from structure coordinates representing the locations of at least the backbone atoms of a plurality of the amino acids defining at least one *S. aureus* peptide deformylase or *S. aureus* peptide deformylase-like active site, the

active site comprising amino acids Gly58, Gly60, Leu61, Gln65, Glu109 , Gly110, Cys111, Leu112, Ile150, His154, Glu155, and His158.

12. The scalable three-dimensional configuration of points of claim 9 wherein at least a portion of the points derived from the *S. aureus* peptide deformylase structure coordinates are derived from structure coordinates representing the locations of at least the backbone atoms of a plurality of the amino acids defining at least one *S. aureus* peptide deformylase or *S. aureus* peptide deformylase-like active site, the active site comprising amino acids Arg56, Ser57, Gly58, Val59, Gly60, Leu61, Gln65, Leu105, Pro106, Thr107, Gly108, Glu109 , Gly110, Cys111, Leu112, Asn117, Tyr147, Ile150, Val151, His154, Glu155, and His158.

13. The scalable three-dimensional configuration of points of claim 9 displayed as a holographic image, a stereodiagram, a model or a computer-displayed image.

14. A scalable three-dimensional configuration of points, at least a portion of the points derived from structure coordinates of at least a portion of a molecule or a molecular complex that is structurally homologous to an *S. aureus* peptide deformylase molecule or molecular complex, wherein the points derived from the structurally homologous molecule or molecular complex have a root mean square deviation of less than about 1.4 Å from the structure coordinates of said structurally homologous complex, and wherein the *S. aureus* peptide deformylase molecule or molecular complex is represented by *S. aureus* peptide deformylase structure coordinates listed in Table 1.

15. The scalable three -dimensional configuration of points of claim 14 displayed as a holographic image, a stereodiagram, a model or a computer-displayed image

16. A machine-readable data storage medium comprising a data storage material encoded with machine readable data which, when using a machine programmed with instructions for using said data, displays a graphical three-dimensional representation of at least one molecule or molecular complex selected from the group consisting of:

(i) a molecule or molecular complex comprising at least a portion of an *S. aureus* peptide deformylase or an *S. aureus* peptide deformylase-like active site comprising amino acids Gly58, Gly60, Leu61, Gln65, Glu109 , Gly110, Cys111, Leu112, Ile150, His154, Glu155, and His158, the active site being defined by a set of points having a root mean square deviation of less than about 0.35 Å from points representing the backbone atoms of said amino acids as represented by structure coordinates listed in Table 1;

(ii) a molecule or molecular complex comprising at least a portion of an *S. aureus* peptide deformylase or an *S. aureus* peptide deformylase-like active site comprising amino acids Arg56, Ser57, Gly58, Val59, Gly60, Leu61, Gln65, Leu105, Pro106, Thr107, Gly108, Glu109 , Gly110, Cys111, Leu112, Asn117, Tyr147, Ile150, Val151, His154, Glu155, and His158, the active site being defined by a set of points having a root mean square deviation of less than about 0.8 Å from points representing the backbone atoms of said amino acids as represented by structure coordinates listed in Table 1; and

(iii) a molecule or molecular complex that is structurally homologous to an *S. aureus* peptide deformylase molecule or molecular complex, wherein the *S. aureus* peptide deformylase molecule or molecular complex is represented by structure coordinates listed in Table 1.

17. A machine-readable data storage medium comprising a data storage material encoded with a first set of machine readable data which, when combined with a second set of machine readable data, using a machine programmed with instructions for using said first set of data and said second set of data, determines at least a portion of the structure coordinates corresponding to the second set of machine

readable data, wherein said first set of data comprises a Fourier transform of at least a portion of the structural coordinates for *S. aureus* peptide deformylase listed in Table 1; and said second set of data comprises an x-ray diffraction pattern of a molecule or molecular complex of unknown structure.

18. A computer-assisted method for obtaining structural information about a molecule or a molecular complex of unknown structure comprising:

crystallizing the molecule or molecular complex;

generating an x-ray diffraction pattern from the crystallized molecule or molecular complex;

applying at least a portion of the structure coordinates set forth in Table 1 to the x-ray diffraction pattern to generate a three-dimensional electron density map of at least a portion of the molecule or molecular complex whose structure is unknown.

19. A computer-assisted method for homology modeling an *S. aureus* peptide deformylase homolog comprising:

aligning the amino acid sequence of an *S. aureus* peptide deformylase homolog with the amino acid sequence of *S. aureus* peptide deformylase SEQ ID NO:1 and incorporating the sequence of the *S. aureus* peptide deformylase homolog into a model of *S. aureus* peptide deformylase derived from structure coordinates set forth in Table 1 to yield a preliminary model of the *S. aureus* peptide deformylase homolog;

subjecting the preliminary model to energy minimization to yield an energy minimized model;

remodeling regions of the energy minimized model where stereochemistry restraints are violated to yield a final model of the *S. aureus* peptide deformylase homolog.

20. A computer-assisted method for identifying a potential modifier of *S. aureus* peptide deformylase activity comprising:

supplying a computer modeling application with a set of structure coordinates of a molecule or molecular complex, the molecule or molecular complex comprising at least a portion of at least one *S. aureus* peptide deformylase or *S. aureus* peptide deformylase-like active site, the active site comprising amino acids Gly58, Gly60, Leu61, Gln65, Glu109 , Gly110, Cys111, Leu112, Ile150, His154, Glu155, and His158;

supplying the computer modeling application with a set of structure coordinates of a chemical entity; and

determining whether the chemical entity is expected to bind to the molecule or molecular complex, wherein binding to the molecule or molecular complex is indicative of potential modification of *S. aureus* peptide deformylase activity.

21. The method of claim 20 further comprising assaying the potential modifier to determine whether it modifies *S. aureus* peptide deformylase activity.

22. The method of claim 20 wherein the active site comprises amino acids Gly58, Gly60, Leu61, Gln65, Glu109 , Gly110, Cys111, Leu112, Ile150, His154, Glu155, and His158, the active site being defined by a set of points having a root mean square deviation of less than about 0.35 Å from points representing the backbone atoms of said amino acids as represented by structure coordinates listed in Table 1.

23. The method of claim 20 wherein determining whether the chemical entity is expected to bind to the molecule or molecular complex comprises performing a fitting operation between the chemical entity and at least one active site of the molecule or molecular complex, followed by computationally analyzing the results of the fitting operation to quantify the association between the chemical entity and the active site.

24. The method of claim 20 further comprising screening a library of chemical entities.

25. A computer-assisted method for identifying a potential modifier of *S. aureus* peptide deformylase activity comprising:

supplying a computer modeling application with a set of structure coordinates of a molecule or molecular complex, the molecule or molecular complex comprising at least a portion of at least one *S. aureus* peptide deformylase or *S. aureus* peptide deformylase-like active site, the active site comprising amino acids Arg56, Ser57, Gly58, Val59, Gly60, Leu61, Gln65, Leu105, Pro106, Thr107, Gly108, Glu109 , Gly110, Cys111, Leu112, Asn117, Tyr147, Ile150, Val151, His154, Glu155, and His158;

supplying the computer modeling application with a set of structure coordinates of a chemical entity; and

determining whether the chemical entity is expected to bind to the molecule or molecular complex, wherein binding to the molecule or molecular complex is indicative of potential modification of *S. aureus* peptide deformylase activity.

26. The method of claim 25 further comprising assaying the potential modifier to determine whether it modifies *S. aureus* peptide deformylase activity.

27. The method of claim 25 wherein the active site comprises amino acids Arg56, Ser57, Gly58, Val59, Gly60, Leu61, Gln65, Leu105, Pro106, Thr107, Gly108, Glu109 , Gly110, Cys111, Leu112, Asn117, Tyr147, Ile150, Val151, His154, Glu155, and His158, the active site being defined by a set of points having a root mean square deviation of less than about 0.8 Å from points representing the backbone atoms of said amino acids as represented by structure coordinates listed in Table 1.

28. The method of claim 25 wherein determining whether the chemical entity is expected to bind to the molecule or molecular complex comprises performing a fitting operation between the chemical entity and at least one active site of the molecule or molecular complex, followed by computationally analyzing the results of the fitting operation to quantify the association between the chemical entity and the active site.

29. The method of claim 25 further comprising screening a library of chemical entities.

30. A computer-assisted method for designing a potential modifier of *S. aureus* peptide deformylase activity comprising:

supplying a computer modeling application with a set of structure coordinates of a molecule or molecular complex, the molecule or molecular complex comprising at least a portion of at least one *S. aureus* peptide deformylase or *S. aureus* peptide deformylase-like active site, the active site comprising amino acids Gly58, Gly60, Leu61, Gln65, Glu109 , Gly110, Cys111, Leu112, Ile150, His154, Glu155, and His158;

supplying the computer modeling application with a set of structure coordinates for a chemical entity;

evaluating the potential binding interactions between the chemical entity and active site of the molecule or molecular complex;

structurally modifying the chemical entity to yield a set of structure coordinates for a modified chemical entity; and

determining whether the modified chemical entity is expected to bind to the molecule or molecular complex, wherein binding to the molecule or molecular complex is indicative of potential modification of *S. aureus* peptide deformylase activity.

31. The method of claim 30 further comprising assaying the potential modifier to determine whether it modifies *S. aureus* peptide deformylase activity.

32. The method of claim 30 wherein the active site comprises amino acids Gly58, Gly60, Leu61, Gln65, Glu109 , Gly110, Cys111, Leu112, Ile150, His154, Glu155, and His158, the active site being defined by a set of points having a root mean square deviation of less than about 0.35 Å from points representing the backbone atoms of said amino acids as represented by structure coordinates listed in Table 1.

33. The method of claim 30 wherein determining whether the modified chemical entity is expected to bind to the molecule or molecular complex comprises performing a fitting operation between the chemical entity and the active site of the molecule or molecular complex, followed by computationally analyzing the results of the fitting operation to quantify the association between the chemical entity and the active site.

34. The method of claim 30 wherein the set of structure coordinates for the chemical entity is obtained from a chemical fragment library.

35. A computer-assisted method for designing a potential modifier of *S. aureus* peptide deformylase activity comprising:

supplying a computer modeling application with a set of structure coordinates of a molecule or molecular complex, the molecule or molecular complex comprising at least a portion of at least one *S. aureus* peptide deformylase or *S. aureus* peptide deformylase-like active site, the active site comprising amino acids Arg56, Ser57, Gly58, Val59, Gly60, Leu61, Gln65, Leu105, Pro106, Thr107, Gly108, Glu109 , Gly110, Cys111, Leu112, Asn117, Tyr147, Ile150, Val151, His154, Glu155, and His158;

supplying the computer modeling application with a set of structure coordinates for a chemical entity;

evaluating the potential binding interactions between the chemical entity and active site of the molecule or molecular complex;

structurally modifying the chemical entity to yield a set of structure coordinates for a modified chemical entity; and

determining whether the modified chemical entity is expected to bind to the molecule or molecular complex, wherein binding to the molecule or molecular complex is indicative of potential modification of *S. aureus* peptide deformylase activity.

36. The method of claim 35 further comprising assaying the potential modifer to determine whether it modifies *S. aureus* peptide deformylase activity.

37. The method of claim 35 wherein the active site comprises amino acids Arg56, Ser57, Gly58, Val59, Gly60, Leu61, Gln65, Leu105, Pro106, Thr107, Gly108, Glu109 , Gly110, Cys111, Leu112, Asn117, Tyr147, Ile150, Val151, Glu155, and His158, the active site being defined by a set of points having a root mean square deviation of less than about 0.8 Å from points representing the backbone atoms of said amino acids as represented by structure coordinates listed in Table 1.

38. The method of claim 35 wherein determining whether the modified chemical entity is expected to bind to the molecule or molecular complex comprises performing a fitting operation between the chemical entity and the active site of the molecule or molecular complex, followed by computationally analyzing the results of the fitting operation to quantify the association between the chemical entity and the active site.

39. The method of claim 35 wherein the set of structure coordinates for the chemical entity is obtained from a chemical fragment library.

40. A computer-assisted method for designing a potential modifier of *S. aureus* peptide deformylase activity *de novo* comprising:

supplying a computer modeling application with a set of structure coordinates of a molecule or molecular complex, the molecule or molecular complex comprising at least a portion of at least one *S. aureus* peptide deformylase or *S. aureus* peptide deformylase-like active site, wherein the active site comprises amino acids Gly58, Gly60, Leu61, Gln65, Glu109 , Gly110, Cys111, Leu112, Ile150, His154, Glu155, and His158;

forming a chemical entity represented by set of structure coordinates; and

determining whether the chemical entity is expected to bind to the molecule or molecular complex, wherein binding to the molecule or molecular complex is indicative of potential modification of *S. aureus* peptide deformylase activity.

41. The method of claim 40 further comprising assaying the potential modifier to determine whether it modifies *S. aureus* peptide deformylase activity.

42. The method of claim 40 wherein the active site comprises amino acids Gly58, Gly60, Leu61, Gln65, Glu109 , Gly110, Cys111, Leu112, Ile150, His154, Glu155, and His158, the active site being defined by a set of points having a root mean square deviation of less than about 0.35 Å from points representing the backbone atoms of said amino acids as represented by structure coordinates listed in Table 1.

43. The method of claim 40 wherein determining whether the modified chemical entity is expected to bind to the molecule or molecular complex comprises performing a fitting operation between the chemical entity and the active site of the molecule or molecular complex, followed by computationally analyzing the results of

the fitting operation to quantify the association between the chemical entity and the active site.

44. A computer-assisted method for designing a potential modifier of *S. aureus* peptide deformylase activity *de novo* comprising:

supplying a computer modeling application with a set of structure coordinates of a molecule or molecular complex, the molecule or molecular complex comprising at least a portion of at least one *S. aureus* peptide deformylase or *S. aureus* peptide deformylase-like active site, wherein the active site comprises amino acids Arg56, Ser57, Gly58, Val59, Gly60, Leu61, Gln65, Leu105, Pro106, Thr107, Gly108, Glu109 , Gly110, Cys111, Leu112, Asn117, Tyr147, Ile150, Val151, His154, Glu155, and His158;

forming a chemical entity represented by set of structure coordinates; and

determining whether the chemical entity is expected to bind to the molecule or molecular complex, wherein binding to the molecule or molecular complex is indicative of potential modification of *S. aureus* peptide deformylase activity.

45. The method of claim 44 further comprising assaying the potential modifier to determine whether it modifies *S. aureus* peptide deformylase activity.

46. The method of claim 44 wherein the active site comprises amino acids Arg56, Ser57, Gly58, Val59, Gly60, Leu61, Gln65, Leu105, Pro106, Thr107, Gly108, Glu109 , Gly110, Cys111, Leu112, Asn117, Tyr147, Ile150, Val151, His154, Glu155, and His158, the active site being defined by a set of points having a root mean square deviation of less than about 0.8 Å from points representing the backbone atoms of said amino acids as represented by structure coordinates listed in Table 1.

47. The method of claim 44 wherein determining whether the modified chemical entity is expected to bind to the molecule or molecular complex comprises performing a fitting operation between the chemical entity and the active site of the molecule or molecular complex, followed by computationally analyzing the results of the fitting operation to quantify the association between the chemical entity and the active site.

48. The method of any of claims 20, 25, 30, 35, 40, or 44 further comprising supplying or synthesizing the potential modifier, then assaying the potential modifier to determine whether it modifies *S. aureus* peptide deformylase activity.

49. A method for making a potential modifier of *S. aureus* peptide deformylase activity, the method comprising chemically or enzymatically synthesizing a chemical entity to yield a potential modifier of *S. aureus* peptide deformylase activity, the chemical entity having been identified during a computer-assisted process comprising supplying a computer modeling application with a set of structure coordinates of a molecule or molecular complex, the molecule or molecular complex comprising at least a portion of a *S. aureus* peptide deformylase or *S. aureus* peptide deformylase-like active site; supplying the computer modeling application with a set of structure coordinates of a chemical entity; and determining whether the chemical entity is expected to bind to the molecule or molecular complex at the active site, wherein binding to the molecule or molecular complex is indicative of potential modification of *S. aureus* peptide deformylase activity.

50. A method for making a potential modifier of *S. aureus* peptide deformylase activity, the method comprising chemically or enzymatically synthesizing a chemical entity to yield a potential modifier of *S. aureus* peptide deformylase activity, the chemical entity having been designed during a computer-assisted process comprising supplying a computer modeling application with a set of structure coordinates of a

molecule or molecular complex, the molecule or molecular complex comprising at least a portion of a *S. aureus* peptide deformylase or *S. aureus* peptide deformylase-like active site; supplying the computer modeling application with a set of structure coordinates for a chemical entity; evaluating the potential binding interactions between the chemical entity and the active site of the molecule or molecular complex; structurally modifying the chemical entity to yield a set of structure coordinates for a modified chemical entity; and determining whether the chemical entity is expected to bind to the molecule or molecular complex at the active site, wherein binding to the molecule or molecular complex is indicative of potential modification of *S. aureus* peptide deformylase activity.

51. A method for making a potential modifier of *S. aureus* peptide deformylase activity, the method comprising chemically or enzymatically synthesizing a chemical entity to yield a potential modifier of *S. aureus* peptide deformylase activity, the chemical entity having been designed during a computer-assisted process comprising supplying a computer modeling application with a set of structure coordinates of a molecule or molecular complex, the molecule or molecular complex comprising at least a portion of a *S. aureus* peptide deformylase or *S. aureus* peptide deformylase-like active site; forming a chemical entity represented by set of structure coordinates; and determining whether the chemical entity is expected to bind to the molecule or molecular complex at the active site, wherein binding to the molecule or molecular complex is indicative of potential modification of *S. aureus* peptide deformylase activity.

52. A potential modifier of *S. aureus* peptide deformylase activity identified or designed according to the method of claims 20, 25, 30, 35, 40, 44, 49, 50, or 51.

53. A composition comprising a potential modifier of *S. aureus* peptide deformylase activity identified or designed according to the method of claims 20, 25, 30, 35, 40, 44, 49, 50, or 51.

54. A pharmaceutical composition comprising a potential modifier of *S. aureus* peptide deformylase activity identified or designed according to the method of claims 20, 25, 30, 35, 40, 44, 49, 50, or 51, or a salt thereof, and pharmaceutically acceptable carrier.

55. A method for crystallizing an *S. aureus* peptide deformylase molecule or molecular complex comprising:

preparing a stock solution of purified *S. aureus* peptide deformylase at a concentration of about 1 mg/ml to about 50 mg/ml;

contacting the stock solution with a precipitating solution containing about 1 % by weight to about 35 % by weight PEG having a number average molecular weight between about 300 and about 20,000; about 0 M to about 0.2 M $MgCl_2$; and about 0 % by weight to about 25 % by weight DMSO; the precipitating solution being buffered to a pH of about 5 to about 9; and

allowing *S. aureus* peptide deformylase to crystallize from the resulting solution.

56. A method for crystallizing an *S. aureus* peptide deformylase molecule or molecular complex comprising:

preparing a stock solution of purified *S. aureus* peptide deformylase at a concentration of about 1 mg/ml to about 50 mg/ml;

contacting the stock solution with a precipitating solution containing about 1 % by weight to about 40 % by weight PEG having a number average molecular weight between about 300 and about 20,000; about 0.005 M to about 0.5 M citric

acid; about 0 % by weight to about 25 % by weight DMSO; and sufficient base to adjust the pH of the precipitating solution to about 5.0 to about 6.5; and

allowing *S. aureus* peptide deformylase to crystallize from the resulting solution.

57. A method for crystallizing an *S. aureus* peptide deformylase molecule or molecular complex comprising:

preparing a stock solution of purified *S. aureus* peptide deformylase at a concentration of about 1 mg/ml to about 50 mg/ml;

contacting the stock solution with a precipitating solution containing about 0.2 M to about 1.5 M sodium citrate; about 0.005 M to about 0.5 M Hepes; about 0 % by weight to about 25 % by weight DMSO; and sufficient base to adjust the pH of the precipitating solution to about 7.0 to about 8.5; and

allowing *S. aureus* peptide deformylase to crystallize from the resulting solution.

58. A method for crystallizing an *S. aureus* peptide deformylase molecule or molecular complex comprising:

preparing a stock solution of purified *S. aureus* peptide deformylase at a concentration of about 1 mg/ml to about 50 mg/ml;

contacting the stock solution with a precipitating solution containing about 1 % by weight to about 40 % by weight PEG having a number average molecular weight between about 300 and about 20,000; about 0 M to about 0.4 M $MgCl_2$; and about 0 % by weight to about 25 % by weight DMSO; the precipitating solution being buffered to a pH of about 7 to about 9; and

allowing *S. aureus* peptide deformylase to crystallize from the resulting solution.

59. Crystalline *S. aureus* peptide deformylase.

60. A crystal of *S. aureus* peptide deformylase having the orthorhombic space group symmetry $C222_1$.

61. A crystal of *S. aureus* peptide deformylase comprising a unit cell having dimensions a, b, and c; wherein a is about 90 Å to about 100 Å, b is about 116 Å to about 128 Å, and c is about 45 Å to about 50 Å; and wherein $\alpha = \beta = \gamma = 90°$.

62. A crystal of *S. aureus* peptide deformylase having the orthorhombic space group symmetry $C222_1$ and comprising a unit cell having dimensions a, b, and c; wherein a is about 90 Å to about 100 Å, b is about 116 Å to about 128 Å, and c is about 45 Å to about 50 Å; and wherein $\alpha = \beta = \gamma = 90°$.

63. A crystal of *S. aureus* peptide deformylase having the space group symmetry C2 and comprising a unit cell having dimensions a, b, and c; wherein a is about 85 Å to about 100 Å, b is about 35 Å to about 50 Å, and c is about 90 Å to about 110 Å; and wherein $\alpha = \gamma = 90°$ and β is about 90° to about 95°.

64. A crystal of *S. aureus* peptide deformylase having the tetragonal space group symmetry $P4_1$ or $P4_22_12$ and comprising a unit cell having dimensions a, b, and c; wherein a and b are about 130 Å to about 190 Å, and c is about 30 Å to about 70 Å; and wherein $\alpha=\beta = \gamma = 90°$.

65. A crystal of *S. aureus* peptide deformylase comprising atoms arranged in a spatial relationship represented by the structure coordinates listed in Table 1.

66. A crystal of *S. aureus* peptide deformylase having a single *S. aureus* peptide deformylase molecule as the asymmetric unit.

67. A crystal of *S. aureus* peptide deformylase having an *S. aureus* peptide deformylase amino acid SEQ ID NO:1.

68. A crystal of *S. aureus* peptide deformylase having a *S. aureus* peptide deformylase amino acid SEQ ID NO:1, except that at least one methionine is replaced with selenomethionine.

69. A crystal of *S. aureus* peptide deformylase having a coordinated metal ion selected from the group of metals consisting of Fe, Zn, Ni and combinations thereof.

09265202 : 060904